Liang Wang

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Education

Institution of Automation, Chinese Academy of Sciences — **Beijing, China**

Ph.D. in Pattern Recognition and Intelligent Systems (selected for the PhD honors program) — *2021 - 2026 (expected)*

- Center for Research on Intelligent Perception and Computing (CRIPAC), State Key Laboratory of Multimodal Artificial Intelligence Systems (MAIS)
- Advisor: Prof. Liang Wang Co-advisors: Prof. Shu Wu and Qiang Liu
- Research Interests: AI for Science, Graph Machine Representation Learning, Data Mining

Tongji University — **Shanghai, China**

B.Eng. in Software Engineering — *2017 - 2021*

- GPA: 4.86/5.00 (Ranking 3/214, Top 1.4%)
- Honors and Awards: National Scholarship (Top 1%), Outstanding Graduate of Shanghai (Top 5%)

Selected Publications

MolSpectra: Pre-training 3D Molecular Representation with Multi-modal Energy Spectra

- Liang Wang, Shaozhen Liu, Yu Rong, Deli Zhao, Qiang Liu, Shu Wu, Liang Wang
- *ICLR 2025*

Pin-Tuning: Parameter-Efficient In-Context Tuning for Few-Shot Molecular Property Prediction

- Liang Wang, Qiang Liu, Shaozhen Liu, Xin Sun, Shu Wu, Liang Wang
- *NeurIPS 2024*

Rethinking Graph Masked Autoencoders through Alignment and Uniformity

- Liang Wang*, Xiang Tao*, Qiang Liu, Shu Wu, Liang Wang
- *AAAI 2024*

DIVE: Subgraph Disagreement for Graph Out-of-Distribution Generalization

- Xin Sun, Liang Wang, Qiang Liu, Shu Wu, Zilei Wang, Liang Wang
- *KDD 2024*

GSLB: The Graph Structure Learning Benchmark

- Zhixun Li, Liang Wang, Xin Sun, Yifan Luo, Yanqiao Zhu, Dingshuo Chen, Yingtao Luo, Xiangxin Zhou, Qiang Liu, Shu Wu, Liang Wang, Jeffrey Xu Yu
- *NeurIPS 2023*

Bi-Level Graph Structure Learning for Next POI Recommendation

- Liang Wang, Shu Wu, Qiang Liu, Yanqiao Zhu, Xiang Tao, Mengdi Zhang, Liang Wang
- *IEEE Transactions on Knowledge and Data Engineering*

Semantic Evolvement Enhanced Graph Autoencoder for Rumor Detection

- Xiang Tao, Liang Wang, Qiang Liu, Shu Wu, Liang Wang
- *WWW 2024*

Chain-of-History Reasoning for Temporal Knowledge Graph Forecasting

- Yuwei Xia, Ding Wang, Qiang Liu, Liang Wang, Shu Wu, Xiaoyu Zhang
- *ACL 2024 (Findings)*

Selected Projects

PyGCL: A PyTorch Library for Graph Contrastive Learning — **https://github.com/PyGCL/PyGCL**

- ☆ Github Star: 919
- An easy-to-use library for graph contrastive learning with PyTorch. It implements a wide variety of contrastive objectives, data augmentations, contrasting modes and other utilities useful for implementing and evaluating contrastive learning on graphs.

GSLB: A Benchmark of Graph Structure Learning — **https://github.com/GSL-Benchmark/GSLB**

- ☆ Github Star: 112
- An open-source library built for easy implementation and evaluation of graph structure learning model family. It offers a versatile control of graph dataset laoding, structure learners, structure processors, and a bunch of reproduced models.

Internship

AI4Science Group, Alibaba DAMO Academy **Hangzhou, China**
Research Intern *Aug. 2024 - Now*

- Advised by Dr. Yu Rong and Tingyang Xu.
- Conducted research on AI for chemistry and life science. The research work has been published in ICLR 2025.

Graph Learning Group, NLP Center, Meituan Inc. **Beijing, China**
Research Intern *Sept. 2021 - Oct. 2022*

- Conducted research on graph self-supervised learning and graph-based spatial-temporal data mining. The research works have been published in IEEE TKDE and SDM 2024.

Advertising Department, ByteDance Inc. **Shanghai, China**
Machine Learning Engineer Intern *Jul. 2020 - Dec. 2020*

- Supported the improvement of advertising machine learning models, and the development of the advertising system.

Talks

Molecular Representation Learning and Property Prediction, Invited by DP Technology, 2024, Slides
Denoising-based 3D Molecular Pre-training, 2024, Slides
Generative Graph Self-Supervised Learning, 2023, Slides
Graph Transformers, 2022, Slides
Graph Self-Supervised Learning and Pre-Training, 2021, Slides

Academic Services

Conference Reviewers: NeurIPS 2024, ICLR 2025, ICML 2025, KDD 2024 2025, AISTATS 2025

Technical Skills

Programming Languages: Python, C++, Matlab, Java, C#
Machine Learning Frameworks: PyTorch, PyTorch Geometric (PyG), Deep Graph Library (DGL)
Others: LaTeX, Git